

Hard squares for $z = -1$

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Abstract

The hard square model in statistical mechanics has been investigated for the case when the activity z is -1 . For cyclic boundary conditions, the characteristic polynomial of the transfer matrix has an intriguingly simple structure, all the eigenvalues x being zero, roots of unity, or solutions of $x^3 = 4 \cos^2(\pi m/N)$. Here we tabulate the results for lattices of up to 12 columns with cyclic or free boundary conditions and the two obvious orientations. We remark that they are all unexpectedly simple and that for the rotated lattice with free or fixed boundary conditions there are obvious likely generalizations to any lattice size.

KEY WORDS: Statistical mechanics, lattice models, transfer matrices.

1 Introduction

The hard square lattice model has long been the subject of study. In 1966 Runnels and Coombs[1] performed numerical calculations on lattices of up to 24 columns (an amazing achievement for the computing power then available). Gaunt and Fisher had previously obtained high and low-density series expansions in 1965[2], and these were extended by Baxter *et al* [3]. For the case $z = +1$, Baxter also calculated the free energy to 43 digits of accuracy using the “corner transfer matrix” technique.[4] Recently Fernandes *et al* have made numerical studies of various hard core two- and three-dimensional systems.[5, 6]

All these calculations naturally focussed on cases of physical interest, when the activity z is real and positive, and were particularly concerned with locating and investigating the critical point at $z \simeq 3.796$, where the system undergoes a transition from a fluid to a solid state. However, as a result of their analysis of the series expansions, Gaunt and Fisher did predict singularities on the negative real axis, at $z \simeq -0.12$ and $z \simeq -3.80$. Between those

values the free energy may have branch cuts or further singularities, and may well be sensitive to the boundary conditions imposed.

Fendley *et al* [7] studied the case when $z = -1$, using the usual cyclic boundary conditions and orientation. For lattices of N columns, with $N \leq 15$, they found that the characteristic polynomial $P_N(x) = \det(xI - T)$ of the row-to-row transfer matrix is remarkable simple, being a product of factors of the form $x^m \pm 1$. This implies that all the eigenvalues of T lie on the unit circle. They conjectured that this behaviour held for lattices of any width.

This conjecture was verified by Jonsson,[8] who established an equivalence between the model and the counting of particular rhombus tilings of the plane. Moreover, he obtained an algorithm for counting these tilings that grows only polynomially (instead of exponentially) with the size of the lattice. He was therefore able to calculate $P_N(x)$ explicitly for lattices of up to 50 columns.

More recently, Jonsson [9] has investigated the effect of first rotating the lattice through 45° before imposing toroidal boundary conditions, and Bousquet-Mélou *et al*[10] have looked at the problem using free boundary conditions. Again they found that $P_N(x)$ is a product of simple factors.

We have explicitly calculated $P_N(x)$ for $N \leq 12$, and for completeness present the results here for the three cases mentioned, plus the remaining case of the 45° orientation with free (or fixed) boundary conditions. This last case is particularly simple, leading us to conjecture its form for general N .

2 The 90° orientation

Fendley *et al* [7] considered the square lattice \mathcal{L} drawn in the obvious way as in Figure 1, with M rows and N columns and $R = MN$ sites. For the hard squares model, with each site i is associated an occupation number σ_i , which takes the values 0 or 1, corresponding to whether the site is empty or contains a particle. At most one particle can lie on any site.

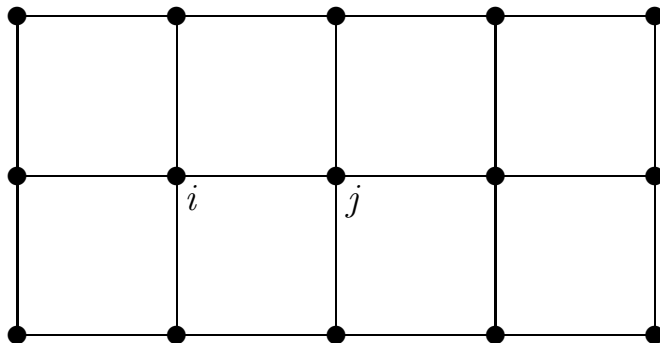


Figure 1: The square lattice of solid lines and circles, showing two adjacent sites i , j .

Particles are also not allowed to occupy adjacent sites. We can express this by defining a weight function $W(\sigma_i, \sigma_j)$ for each edge $\langle i, j \rangle$ of \mathcal{L} by

$$W(a, b) = 1 \text{ if } a, b \text{ not both } 1, \quad (2.1)$$

$$= 0 \text{ if } a = b = 1. \quad (2.2)$$

Let $\boldsymbol{\sigma} = \{\sigma_1, \dots, \sigma_R\}$ denote the set of the occupation numbers of all the sites of \mathcal{L} , and let

$$n(\boldsymbol{\sigma}) = \sum_i \sigma_i, \quad (2.3)$$

the sum being over all the R sites i . Then the partition function is

$$Z_{M,N} = \sum_{\boldsymbol{\sigma}} z^{n(\boldsymbol{\sigma})} \prod_{\langle i,j \rangle} W(\sigma_i, \sigma_j), \quad (2.4)$$

the product being over all edges $\langle i, j \rangle$ of \mathcal{L} and the sum over all values of $\sigma_1, \sigma_2, \dots, \sigma_R$.

Define the partition function per site

$$\kappa = \kappa(z) = (Z_{M,N})^{1/R}. \quad (2.5)$$

The parameter z is known as the *activity*. For real positive values of z we expect $\kappa(z)$ to tend to a positive limit as $M, N \rightarrow \infty$, to be independent of the order in which this occurs, and indeed of the boundary conditions imposed. The free energy or entropy is proportional to $-\log \kappa(z)$ and is the function investigated by Runnels and Coombs,[1] Gaunt and Fisher,[2] and Baxter *et al* [3].

If we impose toroidal boundary conditions, so that row M is followed by row 1, and column N by column 1, then it is straightforward to show that

$$Z_{M,N} = \text{trace } (T_N)^M, \quad (2.6)$$

where T_N is the *transfer matrix*, with entries

$$(T_N)_{\sigma, \sigma'} = \prod_{j=1}^N z^{\sigma_j} W(\sigma_j, \sigma_{j+1}) W(\sigma_j, \sigma'_j) \quad (2.7)$$

where now $\sigma = \{\sigma_1, \dots, \sigma_N\}$, $\sigma' = \{\sigma'_1, \dots, \sigma'_N\}$ and $\sigma_{N+1} = \sigma_1$. The RHS is the combined weight of two adjacent rows of \mathcal{L} , with occupation numbers $\sigma_1, \dots, \sigma_N$ in one row, and $\sigma'_1, \dots, \sigma'_N$ in the row above, as in Figure 2.

As defined here, T_N is a 2^N by 2^N dimensional matrix. However, many of its rows vanish, corresponding to two horizontally adjacent occupation numbers σ_j, σ_{j+1} being both unity. It is natural to exclude such rows and to impose the condition

$$\sigma_j, \sigma_{j+1} \text{ not both one, } j = 1, \dots, N \quad (2.8)$$

on both the sets σ and σ' . This does not change the RHS of (2.6). If S is the two-by-two matrix

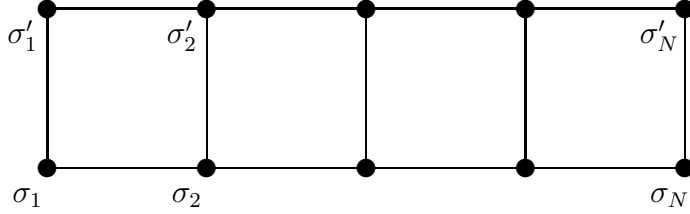


Figure 2: Two rows of \mathcal{L} , corresponding to the element $T_{\sigma, \sigma'}$ of the transfer matrix T .

$$S = \begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix} ,$$

then the matrix T_N is of dimension

$$D_N = \text{trace } S^N .$$

The characteristic polynomial of the matrix T_N is

$$P_N(x) = \det(x I - T_N) . \quad (2.9)$$

For arbitrary values of the activity z , one would not expect this to have any simple structure. However, the case

$$z = -1 \quad (2.10)$$

seems to be very special. Fendley *et al* [7] evaluated $P_N(x)$ for $N = 1, \dots, 15$ and found that it to be amazingly simple, being in each case a product of factors of the form

$$(x^n \pm 1) .$$

Thus all the eigenvalues of T_N lie on the unit circle.

We define the functions

$$f_n = f_n(x) = x^n - 1 , \quad (2.11)$$

and give Fendley *et al*'s results up to $N = 12$ in Table 1. In each case the denominator is a factor of the numerator, so each expression is in fact a polynomial in x , of degree D_N .

N	D_N	$P_N(x)$
1	1	f_1
2	3	$f_1 f_4 / f_2$
3	4	$f_1 f_3$
4	7	$f_1 f_2 f_4$
5	11	$f_1 f_{10}^2 / f_5^2$
6	18	$f_1 f_3 f_4 f_6^2 / f_2$
7	29	$f_1 f_{28}^2 / f_{14}^2$
8	47	$f_1 f_2 f_4 f_{10}^4$
9	76	$f_1 f_3 f_9^4 f_{18}^2$
10	123	$f_1 f_4 f_5^2 f_8^5 f_{14}^5 / f_2$
11	199	$f_1 f_{44}^4 f_{55}^2 / f_{22}^4$
12	322	$f_1 f_2 f_3 f_4 f_6^2 f_{12}^{12} f_{18}^6 f_{24}^2$

Table 1: $P_N(x)$ for the 90° orientation with cyclic boundary conditions.

Free and fixed boundary conditions

One does not have to impose toroidal (i.e. cyclic in both the vertical and horizontal directions) boundary conditions on the lattice \mathcal{L} . Other boundary conditions are of interest in statistical mechanics, in particular cylindrical boundary conditions, where \mathcal{L} begins on the left at column 1 and ends on the right at column N . If one still imposes cyclic boundary conditions from top to bottom (so that row M is followed by row 1), then $Z_{M,N}$ is again given by (2.6) and (2.7), except that the single factor $W(\sigma_N, \sigma_{N+1})$ is omitted.

This is equivalent to requiring that (2.8) hold only for $j = 1, \dots, N-1$, so now T_N is a square matrix of dimension

$$D_N = \sum_{i=1}^2 \sum_{j=1}^2 (S^{N-1})_{i,j} .$$

This case is discussed by Bousquet-Mélou *et al*[10], who calculate $P_N(x)$ for $N = 1, \dots, 10$. We have extended these calculations to $N = 1, \dots, 12$ and give the results in Table 2. Again the denominators are factors of the numerators, so each expression is a polynomial, for instance

$$P_1(x) = x^2 - x + 1 \quad , \quad P_2(x) = (x-1)(x^2+1) \quad .$$

We observe that, surprisingly, these results are similar in form to those for the cyclic case, in particular all the eigenvalues, i.e. the zeros of $P_N(x)$, lie on the unit circle.

We can also consider *fixed boundary conditions*, for instance we could fix $\sigma_1, \sigma_N, \sigma'_1, \sigma'_N$ in (2.7) to be zero. (The factor $W(\sigma_N, \sigma_1)$ is then unity, so it is irrelevant whether it is removed.) However, since then $W(\sigma_1, \sigma_2) = W(\sigma_{N-1}, \sigma_N) = 1$ for all σ_2 and σ_{N-1} , this is merely the same as imposing

N	D_N	$P_N(x)$
1	2	$f_1 f_6 / (f_2 f_3)$
2	3	$f_1 f_4 / f_2$
3	5	$f_1 f_8 / f_4$
4	8	$f_1 f_4 f_6 / f_3$
5	13	$f_1 f_8 f_{10} / (f_2 f_4)$
6	21	$f_1 f_4^2 f_{14} / f_2$
7	34	$f_1 f_6 f_8 f_{12} f_{18} / (f_3 f_4^2)$
8	55	$f_1 f_4^2 f_{16}^2 f_{22} / f_8$
9	89	$f_1 f_8 f_{14} f_{20}^3 f_{26} / (f_2 f_4^2 f_{10})$
10	144	$f_1 f_4^3 f_6 f_{18}^2 f_{24}^3 f_{30} / (f_2 f_3 f_8)$
11	233	$f_1 f_8 f_{14} f_{16} f_{22}^4 f_{28}^3 f_{34} / f_4^3$
12	377	$f_1 f_4^3 f_{10} f_{20}^2 f_{26}^6 f_{32}^4 f_{38} / f_8$

Table 2: $P_N(x)$ for the 90° orientation with free boundary conditions.

free boundary conditions on columns 2 and $N-1$ of \mathcal{L} , so for the 90° orientation

$$[P_N(x)]_{\text{fixed}} = [P_{N-2}(x)]_{\text{free}} \quad . \quad (2.12)$$

3 The 45° orientation

We now consider the square lattice \mathcal{L} turned through 45° , as in Figure 3.

If we sum over the occupation numbers on alternate rows (the solid circles in the figure), then we obtain a new square lattice \mathcal{L}_1 , shown by the open circles and dotted lines in Figure 3, which has the usual 90° orientation used in the previous section. The four sites round a face of \mathcal{L}_1 , e.g. those with occupation numbers a, b, c, d shown, have the weight

$$W_1(a, b, c, d) = \sum_{e=0}^1 z^e W(a, e) W(b, e) W(c, e) W(d, e) \quad . \quad (3.1)$$

Thus

$$W_1(a, b, c, d) = 1 + z \text{ if } a = b = c = d = 0 \quad , \quad (3.2)$$

$$= 1 \quad \text{otherwise} \quad (3.3)$$

and we see that $z = -1$ is special in the sense that $W_1(0, 0, 0, 0)$ then vanishes.

The definition (2.4) is equivalent to

$$Z_{M,N} = \sum_{\boldsymbol{\sigma}} z^{n(\boldsymbol{\sigma})} \prod W_1(\sigma_i, \sigma_j, \sigma_k, \sigma_l) \quad , \quad (3.4)$$

the product being over all faces (i, j, k, l) of \mathcal{L}_1 and the outer sum over all values of the occupation numbers $\boldsymbol{\sigma}$ on \mathcal{L}_1 . Again $n(\boldsymbol{\sigma})$ is defined by (2.3),

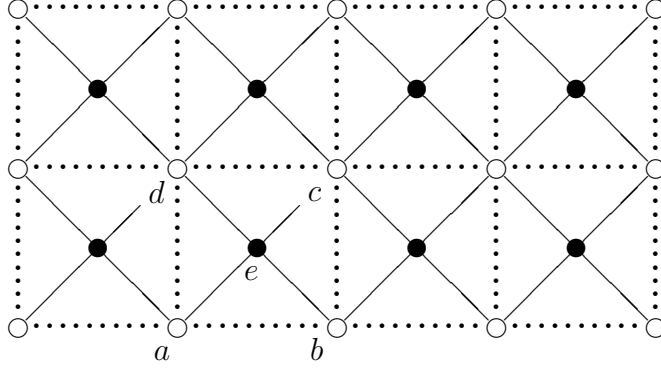


Figure 3: The square lattice \mathcal{L} turned through 45° , indicated by all the circles and the solid lines, and the reduced lattice \mathcal{L}_1 shown by open circles and dotted lines.

but now the sum is over all sites of \mathcal{L}_1 . We now take M, N, R to be the number of rows, columns and sites of \mathcal{L}_1 , so again $R = MN$.

The transfer matrix is no longer given by (2.7), but by

$$(T_N)_{\sigma, \sigma'} = \prod_{j=1}^N z^{\sigma_j} W_1(\sigma_j, \sigma_{j+1}, \sigma'_{j+1}, \sigma'_j) \quad (3.5)$$

and is of dimension 2^N . None of the rows or columns now vanish, but many of the rows of T_N are equal or opposite. This is because two rows with $\sigma = \{a, \dots, b, 1, 0, 1, c, \dots, d\}$ and $\{a, \dots, b, 1, 1, 1, c, \dots, d\}$ must be equal and opposite. (The central occupation number is different, but the face weights on either side are 1 for each of the two cases.) Thus many of the eigenvalues of T_N will be zero, and we do observe this.

For positive integers n , define

$$g_n = g_n(x) = x^3 - n \quad (3.6)$$

If we impose cyclic boundary conditions, so that column N of \mathcal{L}_1 is followed by column 1, then for $z = -1$ and $N = 1, \dots, 12$ we find that the characteristic polynomial $P_N(x)$, as defined by (2.9), is given as in Table 3.

If N is divisible by 3, we see that there are extra factors whose zeros do not in general lie on the unit circle. Nevertheless they do have a simple structure: in each case $P_N(x)$ is a product (or ratio) of factors x, f_n and of

$$s(m, N) = x^3 - 4 \cos^2(\pi m/N) \quad (3.7)$$

To see this, note that $g_4 = s(0, N)$, $g_3 = s(N/6, N)$, $g_2 = s(N/4, N)$, $g_1 = s(N/3, N)$, and

$$x^9 - 6x^6 + 9x^3 - 1 = s(1, 9) s(2, 9) s(4, 9) \quad ,$$

N	D_N	$P_N(x)$
1	2	f_3/f_1
2	4	$x^2 f_3/f_1$
3	8	$x^3 f_1^2 g_4$
4	16	$x^6 f_3 f_4^2/f_1$
5	32	$x^{20} f_3 f_5^2/f_1$
6	64	$x^{44} f_1^2 g_1^2 g_3^2 g_4^2$
7	128	$x^{84} f_3 f_{21}^2/f_1$
8	256	$x^{198} f_3 f_4^2 f_{24}^2/f_1$
9	512	$x^{408} f_1^2 g_1^{12} g_4^4 (x^9 - 6x^6 + 9x^3 - 1)^6$
10	1024	$x^{832} f_3 f_5^2 f_{30}^6/f_1$
11	2048	$x^{1782} f_3 f_{33}^8/f_1$
12	4096	$x^{3660} f_1^2 f_4^2 g_1^{66} g_2^{16} g_3^{18} g_4^{10} (x^6 - 4x^3 + 1)^{16}$

Table 3: $P_N(x)$ for the 45° orientation with cyclic boundary conditions.

$$x^6 - 4x^3 + 1 = s(1, 12) s(5, 12) \quad .$$

This is the case investigated by Jonsson in his second paper[9]. Using the equivalence to rhombus tilings of the plane, he does indeed show that such factors $s(m, N)$ occur when N is divisible by three.

Thus the eigenvalues of T_N lie either at the origin, on the unit circle, or their cubes lie on the interval $(0, 4]$ of the positive real axis.

Free and fixed boundary conditions

As with the 90° case, we can instead impose free boundary conditions, so the factor $W_1(\sigma_N, \sigma_1, \sigma'_1, \sigma'_N)$ (occurring when $j = N$) in the product in (3.5) is omitted. Now we find, for $N = 1, \dots, 12$ that $P_N(x)$ has the very simple forms given in Table 4.

For a given N , define m by

$$m = (4^k - 1)/3 \quad \text{if } N = 3k \quad (3.8)$$

$$= 0 \quad \text{if } N = 3k + 1 \quad (3.9)$$

$$= (1 + 2^{2k+1})/3 \quad \text{if } N = 3k + 2 \quad , \quad (3.10)$$

where k is an integer. Also set

$$r = 1 - \text{mod}(N, 3) \quad , \quad n = 2^N - 3m - r$$

(so $r = 1, 0$ or -1). Then the results of Table 4 are fitted by

$$P_N(x) = [P_N(x)]_{\text{free}} = x^n f_3^m f_1^r \quad . \quad (3.11)$$

As with the 90° orientation, we can also consider *fixed boundary conditions*, in particular by fixing the occupation numbers in the first and last columns

N	D_N	$P_N(x)$
1	2	x^2
2	4	$x^2 f_3 / f_1$
3	8	$x^4 f_1 f_3$
4	16	x^{16}
5	32	$x^{24} f_3^3 / f_1$
6	64	$x^{48} f_1 f_3^5$
7	128	x^{128}
8	256	$x^{224} f_3^{11} / f_1$
9	512	$x^{448} f_1 f_3^{21}$
10	1024	x^{1024}
11	2048	$x^{1920} f_3^{43} / f_1$
12	4096	$x^{3840} f_1 f_3^{85}$

Table 4: $P_N(x)$ for the 45° orientation with free boundary conditions.

of \mathcal{L}_1 to be zero. However, if we go back to the original lattice \mathcal{L} (the solid lines in Figure 3) which has $2N - 1$ columns, this is equivalent to imposing free boundary conditions on columns 2 and $2N - 2$. This means that

$$[Z_{M,N}]_{\text{fixed}} = [Z_{M,N-1}]_{\text{free}} \quad . \quad (3.12)$$

The same relation does not quite hold for the transfer matrices, because T_N for fixed boundary conditions is of dimensions d , while T_{N-1} for free boundaries is of dimensions $2d$, where

$$d = 2^{N-2} \quad . \quad (3.13)$$

For fixed or free boundary conditions we see from Figure 3 that there are two sorts of rows of the original lattice \mathcal{L} : the ones shown as open circles containing N sites per row, and the ones shown as solid circles containing only $N-1$ sites. This ensures that the transfer matrices factor:

$$[T_{N-1}]_{\text{free}} = S_N R_N \quad , \quad [T_N]_{\text{fixed}} = R_N S_N \quad , \quad (3.14)$$

where R_N is a d by $2d$ matrix and S_N is $2d$ by d . This means that d of the eigenvalues of $T_{N-1}(\text{free})$ vanish trivially, while the other d are the same as those of $T_N(\text{fixed})$. Hence

$$[P_N(x)]_{\text{fixed}} = [P_{N-1}(x)]_{\text{free}} / x^d \quad . \quad (3.15)$$

Thus for both orientations the characteristic polynomial for fixed boundary conditions is obtainable from that for free boundary conditions.

4 Conclusions

For cyclic boundary conditions, with either the 45° or 90° orientations, Jons-son has shown that $P_N(x)$ is product or ratio of factors of the form $x, x^m - 1$,

and (for the 45° case with N divisible by three) $x^3 - 4\cos^2(\pi m/N)$. Somewhat remarkably, these properties appear to remain true when we impose free or fixed boundary conditions. In particular, we conjecture that for the 45° free or fixed cases, $P_N(x)$ is a product or ratio only of the simple factors $x, f_1(x), f_3(x)$, being given by (3.11) and (3.15).

For the 90° cyclic case, if we take the limit when M, N become large while remaining co-prime, then $Z_{M,N} = 1$. On the other hand, from our conjecture (3), for the 45° free case, if $N = 3k + 1$, then r, m in (3.11) are both zero, giving

$$Z_{M,N} = 0 \quad . \quad (4.1)$$

From (2.5) κ for these two cases is 1 and 0, so its limit is certainly dependent on the boundary conditions. This can happen, because when $z = -1$ the Boltzmann weights are not all positive.

So $z = -1$ is a very special non-physical case of the hard squares model. Even so, the transfer matrix does then appear to have very intriguing properties.

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